

Abstract Submitted  
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**Study of Atoms and Molecules with Auxiliary-Field Quantum Monte Carlo**<sup>1</sup> WIRAWAN PURWANTO, MALLIGA SUEWATTANA<sup>2</sup>, HENRY KRAKAUER, SHIWEI ZHANG, ERIC J. WALTER, College of William and Mary, VA — We study the ground-state properties of second-row atoms and molecules using the phaseless auxiliary-field quantum Monte Carlo (AF QMC) method.<sup>3</sup> This method projects the many-body ground state from a trial wave function by means of random walks in the Slater-determinant space. We use a single Slater-determinant trial wave function obtained from density-functional theory (DFT) or Hartree-Fock (HF) calculations. The calculations were done with a plane-wave basis and supercells with periodic boundary condition. We investigate the finite-size effects and the accuracy of pseudopotentials within DFT, HF, and AF QMC frameworks. Pseudopotentials generated from both LDA (OPIUM<sup>4</sup>) and HF<sup>5</sup> are employed. We find that the many-body QMC calculations show a greater sensitivity to the accuracy of the pseudopotentials. With reliable pseudopotentials, the ionization potentials and dissociation energies obtained using AF QMC are in excellent agreement with the experimental results.

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<sup>3</sup>S. Zhang and H. Krakauer, Phys. Rev. Lett. **90**, 136401 (2003)

<sup>4</sup><http://opium.sourceforge.net>

<sup>5</sup>I. Ovcharenko, A. Aspuru-Guzik, and W. A. Lester, J. Chem. Phys. **114**, 7790 (2001)

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